**Vibrational effects in electronic structure:**

**Temperature-dependence, zero-point motion, spectral functions**

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Modifications of electronic eigenenergies due to vibrational effects and electron-phonon coupling are sizable in many materials with light atoms. While often neglected, they have been recently computed from first principles using different formalisms, including the perturbation-based Allen-Heine-Cardona (AHC) theory, in the adiabatic or non-adiabatic harmonic approximation.

I will provide an overview of the concepts and formalism, and discuss [1]: the DFT and GW corrections to the diamond bandgap, the latter (0.6 eV) being significantly higher than the former (0.4 eV); the breakdown of the adiabatic AHC theory for infrared-active materials, and fix of this problem in the non-adiabatic AHC theory. Then, focusing on the latter class of materials, I will establish the connection with a simple approach based on a generalized Frohlich Hamiltonian and discuss the near-cancellation between the first-principles Fan and Debye-Waller contributions [2].

Other consequences of interactions, visible in ARPES experiments, are broadening of quasi-particle peaks and appearance of sidebands in the electron spectral function. Migdal selfenergies and spectral functions will be presented for MgO and LiF. The spectral function obtained from the Dyson equation makes errors in the weight and energy of the quasi-particle (QP) peak and phonon-induced sidebands. Only one phonon satellite appears, with an unphysically large energy difference with respect to the QP peak. By contrast, the spectral function from a cumulant treatment is physically better, giving a quite accurate QP energy and several satellites approximately spaced by the LO phonon energy. I will provide a detailed comparison between the first-principles results and those of the Fröhlich Hamiltonian. Such an analysis applies widely to infra-red active materials.

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2. A. Miglio, M. Giantomassi, Y. Gillet, G. Antonius, V. Brousseau, M. Côté, and X. Gonze, in preparation (2018).
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